



TITLE:

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CITATION:

Yoshikawa, M. ...[et al]. Characterization of silicon dioxide films on 4H-SiC (0001) Si, (1-100) M, and (11-20) A faces by cathodoluminescence spectroscopy. Applied Physics Letters 2013, 102(5): 051612.

ISSUE DATE:

2013-02-08

URL:

<http://hdl.handle.net/2433/187954>

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Citation: [Applied Physics Letters](#) **102**, 051612 (2013); doi: 10.1063/1.4791789

View online: <http://dx.doi.org/10.1063/1.4791789>

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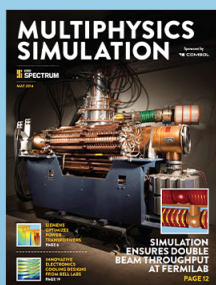
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Characterization of silicon dioxide films on 4H-SiC (0001) Si, (1-100) M, and (11-20) A faces by cathodoluminescence spectroscopy

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(Received 1 December 2012; accepted 29 January 2013; published online 8 February 2013)

We prepared SiO₂ films with channel mobilities (CMs) of 35, 105, and 112 cm²/Vs on 4H-SiC (0001) Si, (1-100) M, and (11-20) A faces by post-oxidation annealing (POA) in NO ambient and measured the cathodoluminescence (CL) spectra. For an acceleration voltage of 5 kV, the CL peak assigned to oxygen vacancy centers (OVCs) weakens by POA, whereas the CL peak related to Si-N bonding structures intensifies with increasing CM. This suggests that OVCs in the SiO₂/SiC interface are terminated by N. We show that NO ambient POA increases the CM more effectively than that by N₂O ambient. CL spectroscopy provides us with extensive information on OVCs, non-bridging oxidation hole centers, and dangling bonds in the SiO₂/SiC interface on 4H-SiC substrates and on the CM in n-type MOS capacitors. © 2013 American Institute of Physics.
[<http://dx.doi.org/10.1063/1.4791789>]

The presence native silicon dioxide in silicon carbide, a well-known wide-bandgap semiconductor, means that SiC is suitable for high-power, high-frequency metal–oxide–semiconductor (MOS) devices. The interface trap densities (D_{it}) at the SiO₂/SiC interface and the effective fixed charge densities (Q_{eff}) are one to two orders of magnitude higher than those typically found at the SiO₂/Si interface (which are of the order of 10¹¹ cm⁻²);¹ these high values degrade the channel mobility (CM).^{2–5} The presence of interface traps in SiC MOS field-effect transistors (FETs) is attributed to (i) excess carbon,^{4,6} (ii) interface defects due to the presence of three-fold coordinated O and C interstitial atoms,^{4,6} and (iii) point defects such as Si and O vacancies that extend into the underlying SiC; this was determined via a comparison with SiO₂ films grown on a Si substrate.^{7,8} Although post-oxidation annealing (POA) by H₂,² NO,^{9,10} or N₂O^{3,11–13} effectively increases the CM, few studies have focused on the effect of POA on the microstructure^{14,15} of SiO₂ films on SiC wafers.

In cathodoluminescence (CL) spectroscopy, luminescence of a sample subjected to electron beam irradiation is observed.^{16–18} CL spectroscopy provides considerable information on the defects in thin SiO₂ films. In a previous study,¹⁹ we measured the CL spectra of SiO₂ films on Si prepared by various methods and observed peaks at 445 and 480 nm, originating from oxygen vacancy centers (OVCs). The CL measurement of the cross section of a thermally grown SiO₂ film on a Si substrate indicated that the intensities of these peaks in the SiO₂/Si interface were stronger than that of the CL peak at 640 nm, which was attributed to non-bridging oxidation hole centers (NBOHCs).¹⁹

We have also measured the CL spectra of SiO₂ films grown on 4H-SiC wafers²⁰ and found that for an acceleration voltage of 5 kV, the CL peaks at 460 and 490 nm assigned to

OVCs become weak after POA in N₂O ambient at 1300 °C, whereas the CL peak around 580 nm related to Si-N bonding structures becomes intense. Furthermore, the peak assigned to N-Si³ configurations in X-ray photoelectron spectroscopy (XPS) spectra was observed in the SiO₂/SiC interface only in samples annealed in N₂O ambient. These results suggested that the D_{it} decreased and the CM in n-type MOS capacitors increased by the termination of dangling bonds by the N atom in the SiO₂/SiC interface. CL spectroscopy and XPS provided us with extensive information on the OVCs and dangling bonds in the SiO₂/SiC interface on the 4H-SiC substrate.

Although it is known that POA in H₂,² NO,^{9,10} or N₂O^{3,11–13} ambient effectively increases CM, few studies have focused on the effect of POA on the microstructure of the SiO₂/SiC interface on SiC wafers. We prepared SiO₂ films grown on 4H-SiC (0001) Si, (1-100) M, and (11-20) A faces by POA in NO ambient at 1250 °C and found that the SiO₂ film grown on the 4H-SiC (11-20) A face had a very large CM of 112 cm²/Vs. To clarify the origin of this high CM, we studied the changes in the CL spectra of these SiO₂ films and clarified the bonding structures near the SiO₂/SiC interface based on the obtained results.

Epitaxial layers (approximately 5 μm thick) were grown by chemical vapor deposition (CVD) on 4° off-axis (0001) Si, (1-100) M, and (11-20) A faces.²¹ After these layers were RCA cleaned, they were thermally oxidized in dry O₂ at 1250 °C before POA in NO ambient at 1250 °C. The samples were then annealed in Ar ambient at 1250 °C. The typical oxide thickness was approximately 41–47 nm. The D_{it} values were estimated from high-(1 MHz) and low-frequency (quasi-static) capacitance–voltage (C–V) curves of n-type MOS capacitors, and the Q_{eff} values were determined from the flatband voltage in the C–V curves. The voltage sweep rate was 0.1 V/s. The thicknesses, oxidation conditions, as well as the D_{it} , Q_{eff} , and CM values of the samples are listed in Table I.

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TABLE I. Thickness, oxidation condition, interface trap densities (D_{it}), effective fixed charge densities (Q_{eff}), and channel mobility of thermally grown SiO_2 films on the 4H-SiC (0001) Si, (1-100) M, and (11-20) A faces (we call those samples Si, M, and A, respectively).

Face	Thickness (nm)	Thermal oxidation condition	Post-oxidation annealing condition	D_{it} ($\text{cm}^2\text{eV}^{-1}$) ($E_c - 0.2$ eV)	Q_{eff} (cm^{-2})	Mobility (cm^2/Vs)
Si	41	1250 °C 60 min	NO anneal 1250 °C, 60 min Ar anneal 1250 °C, 60 min	5.0×10^{11}	1.5×10^{11}	35
A	47	1250 °C 10 min	NO anneal 1250 °C, 60 min Ar anneal 1250 °C, 60 min	3.4×10^{11}	1.8×10^{11}	112
M	45	1250 °C 10 min	NO anneal 1250 °C, 60 min Ar anneal 1250 °C, 60 min	3.6×10^{11}	1.7×10^{11}	105

We used a scanning electron microscope (SEM) with a Schottky-emission-type gun (HITACHI S-4300SE) as the excitation source for the CL measurements.²⁰ The CL signals were collected by an ellipsoidal mirror and optical fiber and detected using a Jobin Yvon HR-320 single monochromator equipped with a charge coupled device (CCD). We recorded the CL spectra at acceleration voltages of 3 and 5 kV at room temperature with a beam current of less than 5 nA.²² To minimize the degradation caused by electron beam irradiation, most CL spectra were measured for 60 s. We repeated the CL measurements of each film three times and obtained reproducible CL spectra. The CL peaks from the optical fiber that was used for a detection of the CL spectra were not observed in our CL system.^{19,20,22}

Figure 1 shows the CL spectra of the SiO_2 films grown on the 4H-SiC (0001) Si, (1-100) M, and (11-20) A faces (we refer to these as samples Si, M, and A, respectively) measured at 3 kV. CL peaks were observed at 460, 490, and 640 nm for the SiO_2 films on the 4H-SiC substrates. The peak and dip in Fig. 1 at around 900 nm are caused by a combination of the overtone by the CL peak at around 500 nm and absorption of the emitted CL by the optical fiber. The CL peaks at 460 and 490 nm were attributed to OVCs, whereas the CL peak at 640 nm was attributed to NBOHCs.^{20,22} The CL peaks at 390 and 540 nm originate from a bound exciton and donor-acceptor pair by the 4H-SiC substrates, respectively. The weak CL peak at around 280 nm is considered to originate from OVCs.¹⁹

Figure 2 shows the CL spectra of the SiO_2 films for samples Si, M, and A, measured at 5 kV. As shown in Figs. 1 and 2, the CL peaks at around 460 and 490 nm are observed strongly when measured at 3 kV, whereas the CL peak around 580 nm for all the samples is observed strongly when measured at 5 kV.

In a previous paper,²⁰ we measured the CL spectra of SiO_2 films grown on the 4H-SiC (0001) Si face and found that

for 5 kV, the CL peaks at 460 and 490 nm, assigned to OVCs, become weak after POA in N_2O ambient at 1300 °C, whereas the CL peak at around 580 nm, related to Si-N bonding structures, becomes intense. Furthermore, the peak assigned to N-Si³ configurations in XPS spectra was observed in the SiO_2/SiC interface only in samples annealed in N_2O ambient. Based upon the results of the previous paper,²⁰ we concluded that the CL peak at 580 nm for all the samples here could be assigned to Si-N bonding structures. The CL peaks at 580 nm cannot be assigned to the second order transition of the weak CL peaks at 280 nm, because the second order peak is generally weaker than the first order one.

A comparison between Figs. 1 and 2 indicates that for all the samples, the CL peak at 460 nm, which is assigned to OVCs, is stronger at 3 kV than at 5 kV, whereas the CL peak at 580 nm, which is assigned to Si-N bonding structures, is stronger at 5 kV than at 3 kV. Monte Carlo simulations indicated that the penetration depths of electrons in thin SiO_2 films at 3 and 5 kV were approximately 30 and 60 nm, respectively. By comparing the penetration depth and sample thickness, the intensity of the CL peak at 580 nm normalized by that of the CL peak at 460 nm is considered to increase in the SiO_2/SiC interface. This suggests that OVCs in the SiO_2/SiC interface are terminated by N after POA in NO ambient at 1250 °C.

The CL spectra of the SiO_2 films were decomposed into six CL peaks with Gaussian line shapes.^{19,23} Figures 3(a) and 3(b) show the CL spectra obtained by fitting the Gaussian line shapes to the CL spectra for samples Si, M, and A, measured at 3 and 5 kV. As seen in Figs. 3(a) and 3(b), the experimental spectra agree well with the composed one. The decomposed peak at 760 nm might originate from the second order transition of the CL peaks at 390 nm.

Figures 4(a) and 4(b) show the relationship between the CM of the SiC-MOSFET and the relative CL intensity at

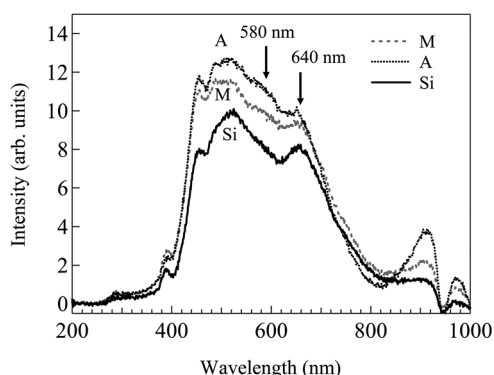


FIG. 1. CL spectra of SiO_2 films on the 4H-SiC (0001) Si, (1-100) M, and (11-20) A faces measured at acceleration voltages of 3 kV.

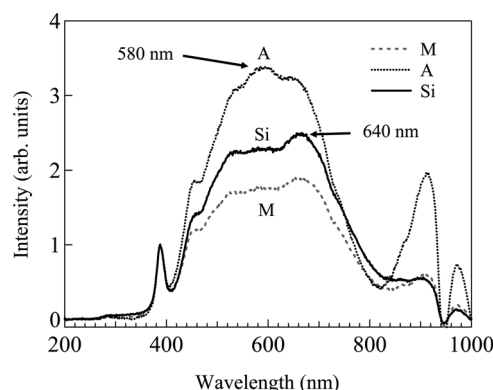


FIG. 2. CL spectra of SiO_2 films on the 4H-SiC (0001) Si, (1-100) M, and (11-20) A faces measured at acceleration voltages of 5 kV.

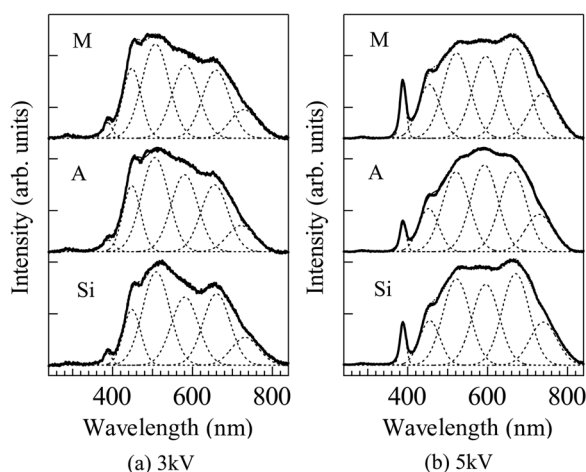


FIG. 3. CL spectra of SiO_2 films on the 4H-SiC (0001) Si, (1-100) M, and (11-20) A faces decomposed into six CL peaks with Gaussian line shapes: (a) 3 and (b) 5 kV. The heavy and solid lines show the experimental and spectra composed by each CL peak decomposed by fitting the Gaussian line shapes to the CL spectra, respectively. The dotted line shows each CL peak decomposed by fitting the Gaussian line shapes to the CL spectra.

580 nm, normalized by that at 460 nm, determined by fitting the Gaussian line shapes to the CL spectra measured at 3 and 5 kV, respectively. As shown in these figures, for sample A with the highest CM of $112 \text{ cm}^2/\text{Vs}$, the relative intensity is stronger at 5 kV than at 3 kV. This shows that the POA decreased the number of OVCs by N termination.

Figures 5(a) and 5(b) show the relationship between the CM of the SiC-MOSFET and the relative CL intensity at 580 nm, normalized by that at 640 nm, measured at 3 and 5 kV, respectively. As shown in Fig. 5, the relative intensity increases in strength in the order of sample Si, M, and A at 3 and 5 kV. This shows that the POA decreased the number of NBOHCs by N termination in the SiO_2/SiC interface in the order of sample Si, M, and A. A comparison between Figs. 4 and 5 suggests that the NO ambient POA tends to decrease the number of OVCs more effectively than NBOHCs in the SiO_2/SiC interface.

We previously measured the CL spectra of SiO_2 films with a CM of $34 \text{ cm}^2/\text{Vs}$ grown on the 4H-SiC Si (0001) face substrate by POA in N_2O ambient at 1300°C and found that the POA decreased the interface trap densities and increased the CM in n-type MOS capacitors by terminating dangling bonds by N in the SiO_2/SiC interface. From a com-

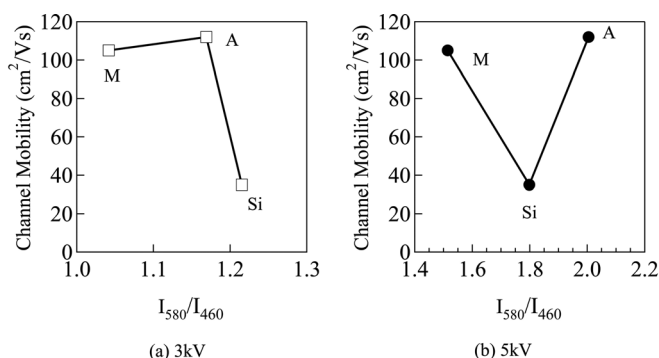


FIG. 4. Relation between the CM of the SiC-MOSFET and the CL relative intensity at 580 nm, normalized by that of 460 nm, measured at an acceleration voltage of (a) 3 and (b) 5 kV.

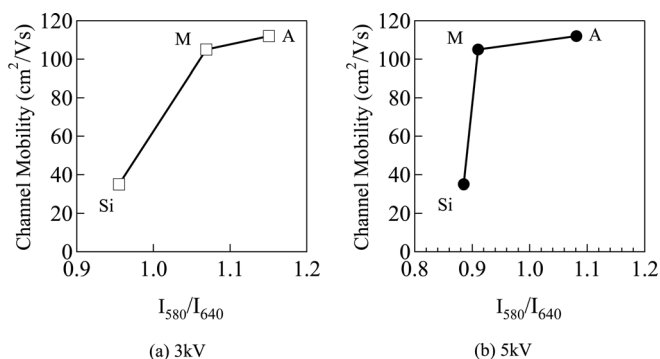


FIG. 5. Relation between the CM of the SiC-MOSFET and the CL relative intensity at 580 nm, normalized by that of 640 nm, measured at an acceleration voltage of (a) 3 and (b) 5 kV.

parison between the previously measured CMs and those in this work, we concluded that the POA in NO ambient at 1250°C decreased the number of OVCs by termination by N in the SiO_2/SiC interface and that the POA in NO ambient increases the CM more effectively than that in N_2O ambient. CL spectroscopy provides us with extensive information on OVCs, NBOHCs, and dangling bonds in the SiO_2/SiC interface on 4H-SiC substrates and on the CM in n-type MOS capacitors.

In summary, we have measured the CL spectra of SiO_2 films grown on 4H-SiC (0001) Si, (1-100) M, and (11-20) A faces and found that for 5 kV, the CL peak at 460 nm, assigned to OVCs, became weak by POA in NO ambient at 1250°C , whereas the CL peak at around 580 nm, related to Si-N bonding structures, became intense, increasing in the order of SiO_2 films grown on 4H-SiC (0001) Si, (1-100) M, and (11-20) A faces. This suggests that OVCs in the SiO_2/SiC interface are terminated by N by NO ambient POA. From a comparison between the CMs in previous work and this work, we concluded that the NO ambient POA decreased the number of OVCs in the SiO_2/SiC interface by N termination and that the NO ambient POA increases the CM more effectively than that in N_2O ambient. CL spectroscopy provides us with extensive information on OVCs, NBOHCs, and dangling bonds in the SiO_2/SiC interface on 4H-SiC substrates and on the CM in n-type MOS capacitors.

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